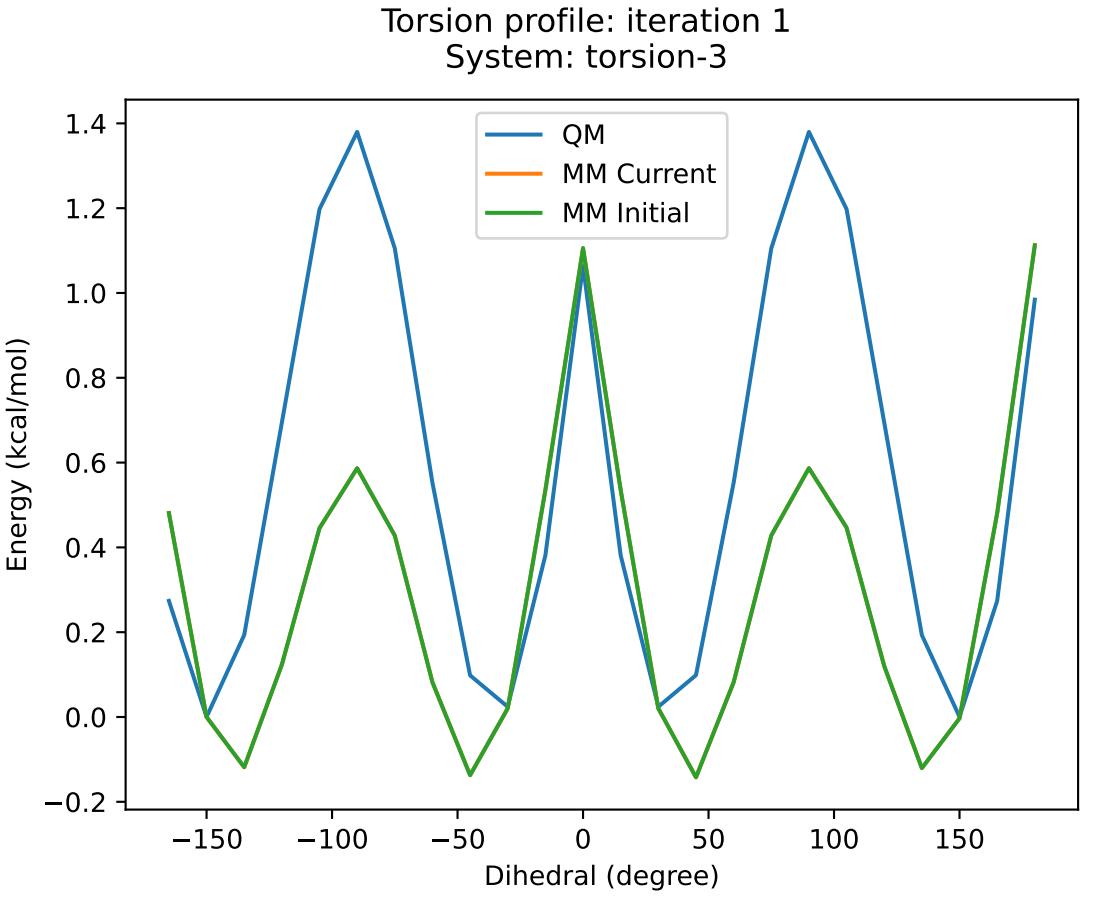
Torsion profile: iteration 1
System: torsion-3
QM
MM Current
MM Initial
Energy (kcal/mol)
Dihedral (degree)
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−150
−100
−50
0
50
100
150